Predicting the Atomic Structures of Defects in Solids

Defects are a universal, unavoidable feature of solid materials, controlling properties and performance in most functional devices (including solar cells, LEDs, transistors, thermoelectrics and batteries). Recent years have seen a dramatic acceleration in the design and development of functional materials, thanks in many parts to powerful combinations of experimental measurements and computational modelling predictions.[1]

The standard approach of modelling defects is, however, prone to obtaining inaccurate results in certain cases. This can occur when the atoms around the defect rearrange in a way that lowers their energy, which can be difficult to predict and identify with our current state-of-the-art computational methods. These rearranged defects can be crucial to the overall behaviour and effect on the material properties, hindering the accuracy (and effectiveness) of defect research. While this issue has been witnessed as far back as 4 decades ago,[2] and attempts made to tackle it,[3,4] a general and affordable method to account for this behaviour has eluded researchers until now.

In this work, we develop a novel method to efficiently 'search' for these defect rearrangements, involving targeted atomic bond distortions, and demonstrate its effectiveness, generality and affordability by applying it to a wide range of solid materials (from the prototype semiconductor silicon, to industry-relevant insulators and ionic oxides such as cerium dioxide, and many others in-between).[5,6] We show that these reconstructions are more common than previously believed, and that they can be crucial to material performance.[6,7] We have developed a computational program to implement our method (ShakeNBreak),[8] and are confident it will provide a significant step forward for accurate quantitative modelling of defects in solids.

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